SACADA Database Code: 254

Topology: 3^6T6

# of independent nodes (IN): 6
Transitivity: [6864]
Space Group: Pm-3m
Pearson: cP176
Coordination Number (CN): 3

Year: 2014

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
3^6T6 (SACADA #254)		1.136		0.788	118.4	52.7	7.3	SACADA[1]
6-1-1-P		1.16	Metal					doi: 10.1016/j.carbon.2014.04.077
6-1-1-P			Semimetal					doi: 10.1103/PhysRevB.92.045108

Elasticity tensor (kBar)[1]

1622.2372	964.9543	964.9543	-0.0000	0.0000	0.0000
964.9543	1622.2372	964.9543	0.0000	-0.0000	-0.0000
964.9543	964.9543	1622.2372	-0.0000	-0.0000	0.0000
0.0000	0.0000	-0.0000	723.1128	0.0000	0.0000
0.0000	-0.0000	-0.0000	0.0000	723.1128	0.0000
0.0000	-0.0000	-0.0000	0.0000	0.0000	723.1128

[1] We apply the density functional theory (DFT) approach by using the Vienna Ab Initio Simulation Package (VASP) to calculate the total energy and properties of carbon allotropes.

DFT calculations

We apply the density functional theory (DFT) approach by using the Vienna Ab Initio Simulation Package (VASP) package [6] to calculate the total energy of carbon allotropes. The Generalized Gradient Approximation [7] (GGA) for exchange-correlational functional is used everywhere. The energy cutoff set to 600 eV. Fully automatic Γ-centered k-points mesh with a reciprocal-space resolution of $2\pi \times 0.025$ Å^{-1} is applied. We used tetrahedron method with Blöchl corrections to perform the k-point integration. The convergence thresholds are set at 10^{-6} eV for energy and 10^{-5} eV Å^{-1} for ionic forces. Polycrystalline elastic moduli — the bulk modulus, the shear modulus, Young's modulus, and the Poisson's ratio ν — have been calculated within the Voigt–Reuss–Hill [8] approximation. The Vicker's hardness H_v has been estimated according to Oganov's model [9].